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Pair distribution functions of the two-dimensional electron gas with two symmetric valleys

M Marchi[1,2], **S De Palo**[1,3], **S Moroni**[1,2] **and G Senatore**[1,3]

[1] INFM-CNR DEMOCRITOS National Simulation Center, Trieste, Italy
[2] SISSA, International School for Advanced Studies, via Beirut 2-4, 34014 Trieste, Italy
[3] Dipartimento di Fisica Teorica, Università di Trieste, Strada Costiera 11, 34014 Trieste, Italy

E-mail: marchi@sissa.it

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Abstract
We present component-resolved and total pair distribution functions for a 2DEG with two symmetric valleys. Our results are based on quantum Monte Carlo simulations performed at several densities and spin polarizations.

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1. Introduction

A two-valley (2V) two-dimensional (2D) electron gas (EG) is the simplest model to describe electrons confined in solid state devices such as Si-MOSFETs [1] and certain quantum wells [2]. In this 2D model, electrons interact via a $1/r$ potential in a uniform neutralizing background and possess an additional discrete degree of freedom (the valley index). One may identify electrons with given spin projection and valley index as belonging to a different species or *component*. We focus on the case of two symmetric valleys, where the number of up- (down-) spin electrons is the same for both valleys. In this case at zero temperature the 2DEG is completely characterized in terms of the coupling parameter $r_s = 1/\sqrt{\pi n} a_B$ and the spin polarization $\zeta = (n_\uparrow - n_\downarrow)/n$ (where n is the total electron density, a_B the Bohr radius, $n_{\uparrow(\downarrow)}$ the density of up- (down-) spin electrons).

The interest in the properties of the 2DEG has been strongly revived in recent years due to the experimental discovery of a previously unexpected metal–insulator transition [3, 4] in which the valley degree of freedom appears to play an important role [5, 6]. The transition takes place at low density, where an accurate treatment of electron correlation is crucial. In this respect, quantum Monte Carlo (QMC) simulations have provided over the years the method of choice for microscopic studies [7–13] of the 2DEG.

We have recently provided an analytic expression of the correlation energy of the 2V2DEG [14]. Here, we focus on the pair distribution functions (PDFs), which are strictly related to the description of exchange and correlation properties of the system (see e.g. [15]). As pointed

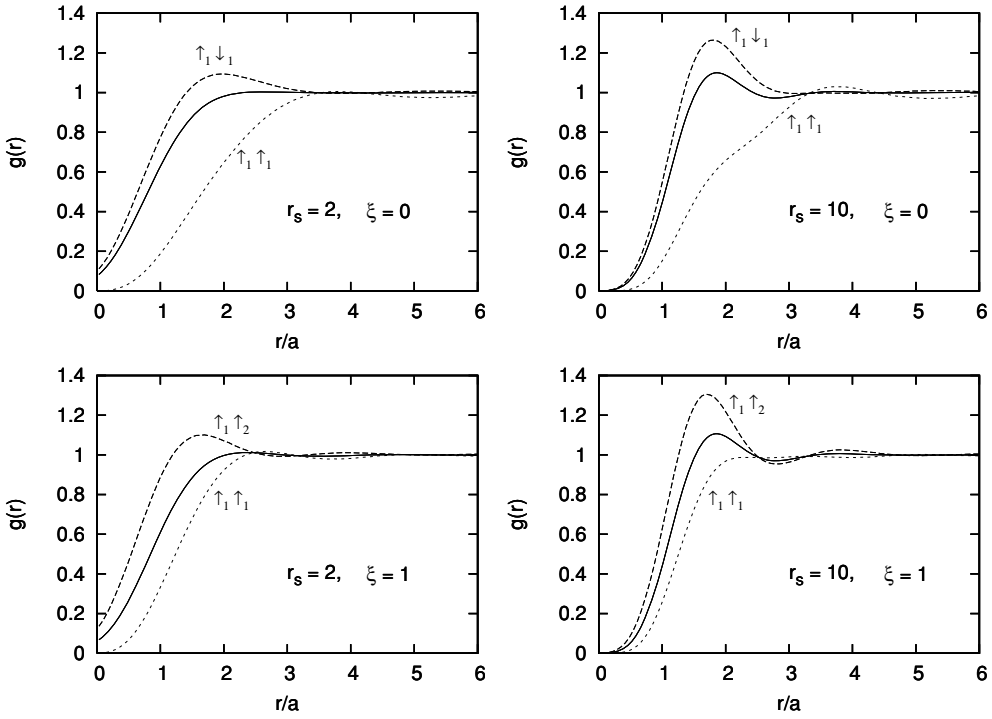

Figure 1. 2V component-resolved pair distribution functions for $\zeta = 0, 1$ and $r_s = 2, 10$. Solid lines represent the total $g(r)$.

out in [13], PDFs may serve a variety of purposes, among which are the estimate of finite thickness effects on the 2DEG spin susceptibility [16], applications in DFT calculations or a test of the accuracy of hypernetted-chain calculations [17].

2. Pair distribution function: definitions

The PDF is related to the probability of finding two electrons at positions $\mathbf{r}$ and $\mathbf{r}'$, respectively. The *component-resolved* PDF $g_{\alpha\beta}(\mathbf{r}', \mathbf{r})$ of a multicomponent 2DEG is defined as [15]

$$g_{\alpha\beta}(\mathbf{r}', \mathbf{r}) = \frac{\left\langle \psi^\dagger_\beta(\mathbf{r}')\psi^\dagger_\alpha(\mathbf{r})\psi_\alpha(\mathbf{r})\psi_\beta(\mathbf{r}')\right\rangle}{n_\beta(\mathbf{r}')n_\alpha(\mathbf{r})} \tag{1}$$

with $\psi^\dagger_\alpha$, ψ_α denoting creation and annihilation field operators, $\langle\cdots\rangle$ the expectation value on the ground state and $n_\alpha(\mathbf{r}) = \left\langle \psi^\dagger_\alpha(\mathbf{r})\psi_\alpha(\mathbf{r})\right\rangle$ the electron density of the component α. The normalization is such that $g_{\alpha\beta} \equiv 1$, in case there is neither exchange nor correlation. In an homogeneous and isotropic system, $g_{\alpha\beta}$ depends only on the relative distance $r = |\mathbf{r} - \mathbf{r}'|$ and there is symmetry for index permutations ($g_{\alpha\beta} = g_{\beta\alpha}$). If $c_\alpha = n_\alpha/n$ is the concentration of the component α, the total (*component-summed*) PDF $g(r)$ reads

$$g(r) = \sum_{\alpha\beta} c_\alpha c_\beta g_{\alpha\beta}(r). \tag{2}$$

In the 2V2DEG, $\alpha \equiv \sigma\nu$ is a composite index which denotes the spin and valley (respectively σ and ν) degrees of freedom and spans the four cases $\alpha = \uparrow 1, \downarrow 1, \uparrow 2, \downarrow 2$.

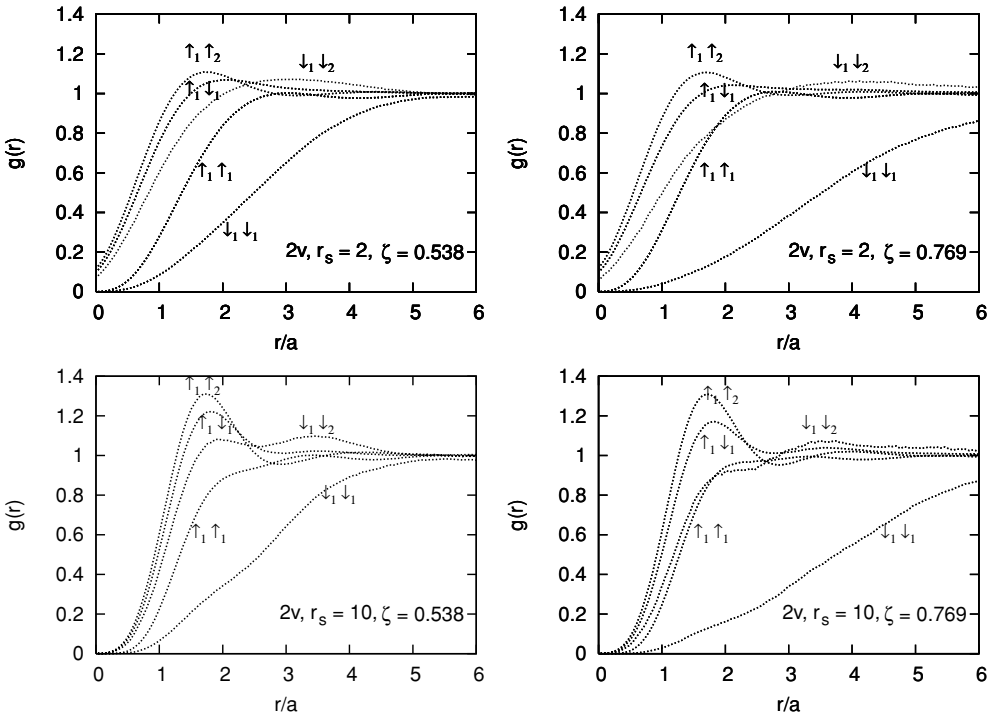

Figure 2. Examples of 2V component resolved pair distribution functions at finite ζ. See labels.

In general, for 2V there are ten different $g_{\alpha\beta}$, but in the case of two symmetric valleys the number of different $g_{\alpha\beta}$ is two for $\zeta = 0, 1$ and five for $0 < \zeta < 1$ (see also [17]). In the following we shall denote the different $g_{\alpha\beta}$ with one of the possible different labels (e.g. for $0 < \zeta < 1 g_{\uparrow 1\downarrow 1} = g_{\uparrow 2\downarrow 2} = g_{\uparrow 1\downarrow 2} = g_{\uparrow 2\downarrow 1}$).

3. Simulation details

Most of the simulation details are the same as in [14]. We performed fixed-phase DMC simulations (for a review of QMC techniques see e.g. [18]) for $r_s = 1, 2, 5, 10, 20$ and $\zeta = 0, 3/13, 5/13, 7/13, 10/13, 1$. To reduce the finite size effects, we used twist-averaged boundary conditions (TABC) [19], which also allow us to change ζ by flipping any number of spins at fixed number of electrons N. To sample the PDFs we performed simulations for a system of $N = 52$ electrons. Time steps were chosen at the different r_s to give an acceptance rate corresponding to $\sim 99\%$. We did simulations with 320 walkers. The twist grid is the same as in [14]. As in [14], we used a Slater–Jastrow trial wave function Ψ_T, but, here, we considered only plane-wave nodes, since the more accurate backflow (BF) nodes yield only slight modifications to the PDFs [8, 13]. Besides, BF effects on the energy were shown to be bigger in the two-component case than in the four-component system [14].

DMC provides the mixed estimate of an operator O, i.e. $\langle O\rangle_{\rm mix} = \langle\Psi_0|O|\Psi_T\rangle/\langle\Psi_0\Psi_T\rangle$ (with Ψ_0 denoting the ground state of the system). If O commutes with the Hamiltonian H, $\langle O\rangle_{\rm mix}$ coincides with the expectation value on the true ground state Ψ_0. If O does not commute with H (as in the case here considered), it is better to compute the extrapolated

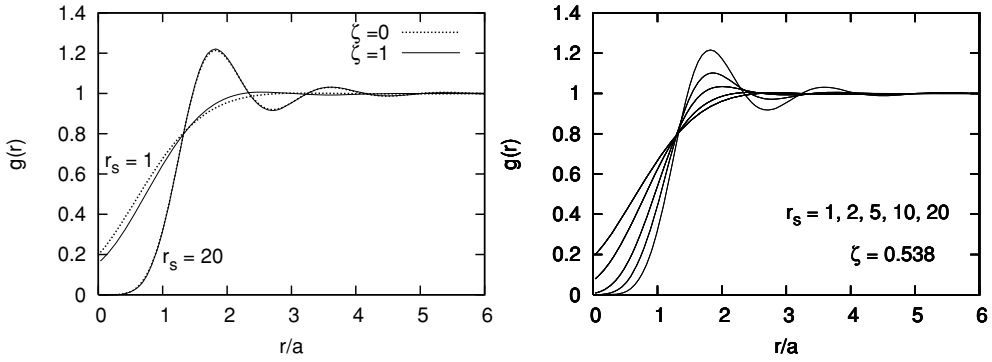

Figure 3. 2V total pair distribution functions. Left panel: $r_s = 1, 20$ and $\zeta = 0, 1$. Right panel: $r_s = 1, 2, 5, 10, 20$ and $\zeta = 0.538$ (increasing peaks for increasing r_s). All lengths are in units of $a = r_s a_B$.

estimate $\langle O\rangle_{\rm extr} = 2\langle O\rangle_{\rm mix} - \langle O\rangle_{\rm VMC} + O(\delta^2)$ (where $\langle O\rangle_{\rm VMC}$ is the variational MC expectation value on Ψ_T) which is accurate to second order in the difference δ between Ψ_0 and Ψ_T.

4. Two valley pair distribution functions

In figures 1 and 2 we show representative examples of 2V component-resolved PDFs for $\zeta = 0, 1$ and finite ζ, respectively. All lengths are given in units of $a = r_s a_B$. The component-resolved PDFs shown in figure 1 illustrate the tendency to a local order which favors electrons belonging to different species (as e.g. $\uparrow$ 1 and $\downarrow$ 1) to get closer than electrons belonging to the same species. For intermediate spin polarizations (see figure 2) the component-resolved PDFs exhibit a richer structure than the $\zeta = 0, 1$ cases, with qualitative features clearly related to the interplay of exchange and correlations (for example, in the density range considered the diagonal PDF of the minority component in a strongly polarized system is found to be determined by exchange alone, to a very good approximation). The significant spin-polarization dependence seen in the component-resolved PDFs almost disappears in the total PDFs, particularly at large r_s. This can be appreciated in figure 3 (left panel), which shows the total PDFs for a high-density ($r_s = 1$) and a low-density ($r_s = 20$) case with zero and full spin polarization. The dependence of the total PDF on r_s is depicted in figure 3 for $\zeta = 0.538$.

We see that even for r_s as small as 1 the effect of exchange on the total PDF, which is expected to decrease with the number N_c of (equally populated) components, is already very small for $N_c = 2$.

Full tabulations of the calculated PDFs are available upon request from the first author.

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